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http://www.cas.org/ONLINE/DBSS/registryss.html

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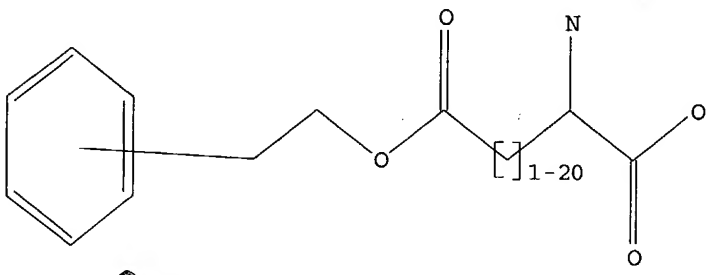
L1 STR



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=> s l2
L3          92 L2

=> s l3 and salt
        714335 SALT
L4            9 L3 AND SALT

=> s l3 and sulfonate
         52599 SULFONATE
L5            0 L3 AND SULFONATE

=> d l4 1-9 sub bib abs
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SIBIB ------- IBIB, no citations

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HITSEQ ------ HIT RN, its text modification, its CA index name, its
structure diagram, plus NTE and SEQ fields
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its structure diagram
FHITSEQ ----- First HIT RN, its text modification, its CA index name, its
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L4 ANSWER 1 OF 9 CA COPYRIGHT 2004 ACS on STN
AB The invention relates to a method for the identification of enzymes that are preferentially expressed in certain tumor tissue as compared with rapidly growing normal cells or tissue and the use of the enzymes to design compds. which generate active anticancer substances selectively in tumor tissue. Compds. X-Y-Q [X is a pro-moiety that is designed to generate an active anticancer substance (Q-Y-H) selectively in tumors by the enzymes; Q-Y- is a radical derived from the active anticancer substance in which Y is O, S or N] and their pharmaceutically-acceptable

salts are claimed. Thus, 13α-[(2R,3S)-2-[(5S)-[5-[(2S)-(2-aminopropionyl)amino]-5-hydroxycarbonyl]pentanoyloxy]-3-(benzoylamino)-3-phenylpropionyloxy]-2a-(benzyloxy)-4a,10β-diacetoxy-1β,7β-dihydroxy-5β,20-epoxytax-1-en-9-one formic acid **salt** (I) was prepared by reaction of taxol with (2S)-2-[(2S)-2-(benzyloxycarbonylamino)-3-phenylpropionylamino]hexanedioic acid 1-benzyl ester. Compound I showed cytotoxicity IC50 = 51 nM after 24 h against human colon cancer cell line HCT116.

AN 139:7174 CA
TI Method for identification of tumor targeting enzymes for design of compounds which generate anticancer substances
IN Ishitsuka, Hideo; Okabe, Hisafumi; Shimma, Nobuo; Tsukuda, Takuo; Umeda, Isao
PA F. Hoffmann-La Roche A.-G., Switz.
SO PCT Int. Appl., 118 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2003043631	A2	20030530	WO 2002-EP12911	20021118
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
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US 2003138864	A1	20030724	US 2002-301460	20021121
PRAI EP 2001-127401	A	20011123		
EP 2001-130245	A	20011219		
EP 2002-5298	A	20020312		

OS MARPAT 139:7174

L4 ANSWER 2 OF 9 CA COPYRIGHT 2004 ACS on STN
AB Motuporin (I) was prepared by a convergent synthesis in which all stereocenters are derived from common amino acids or from D-mandelic acid; the 3 unusual amino acids in I are all derived from D-threonine.
AN 124:30333 CA
TI Enantiospecific total synthesis of the protein phosphatase inhibitor motuporin.
AU Valentekovich, Robert J.; Schreiber, Stuart L.
CS Department of Chemistry, Harvard University, Cambridge, MA, 02138, USA
SO Journal of the American Chemical Society (1995), 117(35), 9069-70
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English
OS CASREACT 124:30333

L4 ANSWER 3 OF 9 CA COPYRIGHT 2004 ACS on STN
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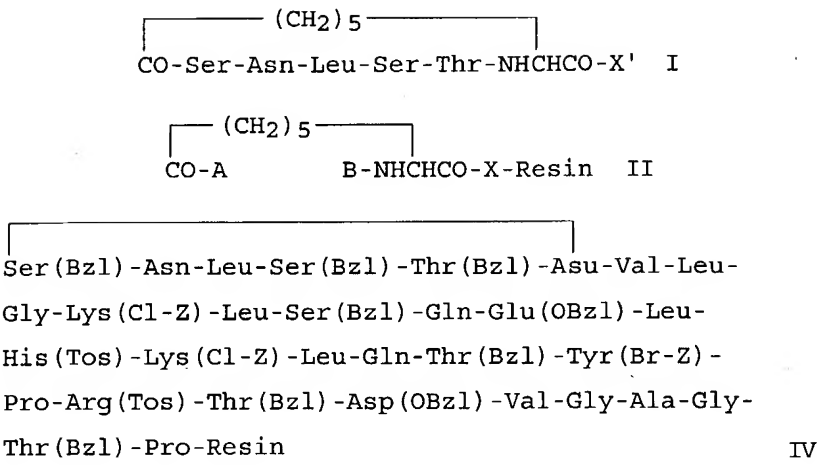

AB Cyclopeptides (I; X1 = OH, NH2, amino acid or peptide residue, wherein each amino acid residue may be protected) are prepared by cyclization of resin-bound open chain peptides [II; A = Ser(X1)-Asn-Leu-Ser(X1)-Thr(X1)-X2, Ser(X1)-Asn-Leu-Ser(X1)-X2, Ser(X1)-Asn-Leu-X2, Ser(X1)-Asn-X2, Ser(X1)-X2; B = X3, X3-Thr(X1), X3-Ser(X1)-Thr(X1), X3-Leu-Ser(X1)-Thr(X1), X3-Asn-Leu-Ser(X1)-Thr(X1); X1 = H, HO-protective group; X3 = H, H2N-protective group; X = direct bond to Resin, amino acid or peptide residue; Resin = resin for solid phase reaction] without using protease followed by resin cleavage. The cyclization proceeds in high yields without side reactions and gives calcitonin derivs., particularly elcatonin, in good yields. Thus, 620 mg R-Leu-Ser(Bzl)-Thr(Bzl)-Asu[Ser(Bzl)-Asn-OR1]-Val-Leu-Gly-Lys(Cl-Z)-Leu-Ser(Bzl)-Gln-Glu(OBzl)-Leu-His(Tos)-Lys(Cl-Z)-Leu-Gln-Thr(Bzl)-Tyr(Br-Z)-Pro-Arg(Tos)-Thr(Bzl)-Asp(OBzl)-Val-Gly-Ala-Gly-Thr(Bzl)-Pro-p-methylbenzhydrylamine polystyrene resin (III; R = Boc, Asu = 2-aminosuberic acid residue, R1 = CMe3, Bzl = CH2Ph, Cl-Z = 2-chlorobenzyloxycarbonyl) (preparation given) was stirred with 50% CF3CO2H in CH2Cl2 at room temperature for 30 min followed by washing with CH2Cl2, 10% (Me2CH)2NEt in DMF, and DMF, III (R = R1 = H) which was added to N-methylpyrrolidone and treated with 1-hydroxybenzotriazole monohydrate and DCC at room temperature for 24 h to give resin bound protected cyclopeptide (IV; Resin = p-methylbenzhydrylamine polystyrene resin). The latter peptide was treated with HF(l) and anisole at 0° for 1 h, distilled in vacuo, washed with Et2O, and extracted with 1 M aqueous AcOH solution; the extract was lyophilized to give 260 mg crude elcatonin which was purified by ion exchange chromatog. and reversed phase HPLC using TSK Gel ODS-120 column (Toso Inc., Ltd.) and **salt** exchange to give elcatonin AcOH **salt**.

AN 122:106541 CA

TI Preparation of cyclic peptides containing α-aminosuberic acid as calcitonin derivatives

IN Inoe, Takashi; Kimura, Hitoshi

PA Daicel Chem, Japan

SO Jpn. Kokai Tokkyo Koho, 15 pp.
CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 06157593	A2	19940603	JP 1992-339821	19921125

PRAI JP 1992-339821 19921125

OS CASREACT 122:106541; MARPAT 122:106541

L4 ANSWER 4 OF 9 CA COPYRIGHT 2004 ACS on STN
AB Two approaches to the synthesis of 2'-O-(N-alkylsuccinamoyl) erythromycin derivs. are explored as a means of introducing anionic and cationic functionalities into erythromycin at the 2'-O-position. The phenacyl group was used to protect the anionic functionality during the synthesis of 2'-O-[N-(carboxylatomethyl)succinamoyl] erythromycin and disodium 2'-O-[N-(1,3-dicarboxylatopropyl)succinamoyl] erythromycin, deprotection being achieved using sodium thiophenoxide under anhydrous conditions. 2'-O-(N-[2-Dimethylammonio)ethyl]succinamoyl] erythromycin lactobionate and (S)-2'-O-[N-(1-methoxycarbonyl-3-guanidinopropyl)succinamoyl] erythromycin required no protection and were prepared in an otherwise similar fashion by mixed anhydride activation of 2'-O-(3-carboxypropanoyl) erythromycin, followed by treatment with the appropriate alkylamine. Sodium 2'-O-[N-(2-sulfonatoethyl)succinamoyl] erythromycin, disodium 2'-O-[N-(1-carboxylato-2-sulfonatoethyl)succinamoyl] erythromycin and trisodium 2'-O-[N-(1-carboxylato-2-phosphonatoethyl)succinamoyl] erythromycin were prepared in a different fashion by treatment of activated 2'-O-(3-carboxypropanoyl) erythromycin with the appropriate amino acid in a Schotten-Baumann related procedure. The aqueous solubilities of derivs. in 0.1 M phosphate buffer are reported along with some preliminary stability information.
AN 115:72090 CA
TI Approaches to novel water-soluble prodrugs of erythromycin A. Synthesis of 2'-O-(N-alkylsuccinamoyl)erythromycin derivatives incorporating anionic and cationic groups
AU Ackland, Mark J.; Atkins, Paul J.; Jones, Norman B.
CS Upjohn Lab.-UK, Upjohn Ltd., Crawley/West Sussex, RH10 2NJ, UK
SO Journal of Chemical Research, Synopses (1991), (6), 142-3
CODEN: JRPSDC; ISSN: 0308-2342
DT Journal
LA English

L4 ANSWER 5 OF 9 CA COPYRIGHT 2004 ACS on STN
AB Human proinsulin C-peptide was synthesized by the solid-phase method. The product was purified consecutively by gel filtration, DEAE-cellulose chromatog., and high-performance liquid chromatog. (HPLC). The purified material behaved as a single component in reversed-phase HPLC, gave correct amino acid ratios, and was not distinguished from natural human C-peptide in terms of immunoreactivity and chromatog. behaviors. The α→β transpeptidation at the Asp-Leu sequence, possible to occur associated with the HF cleavage, was studied using model peptides to demonstrate that the formation of β-peptide was 3-4% regardless of whether the β-carboxylic acid is free or protected as a benzyl ester.
AN 96:52660 CA
TI A synthesis of human proinsulin C-peptide
AU Igano, Kenichi; Minotani, Yuriko; Yoshida, Nobuo; Kono, Masao; Inouye, Ken
CS Shionogi Res. Lab., Shionogi Co., Ltd., Osaka, 553, Japan
SO Bulletin of the Chemical Society of Japan (1981), 54(10), 3088-94
CODEN: BCSJA8; ISSN: 0009-2673
DT Journal
LA English

L4 ANSWER 6 OF 9 CA COPYRIGHT 2004 ACS on STN
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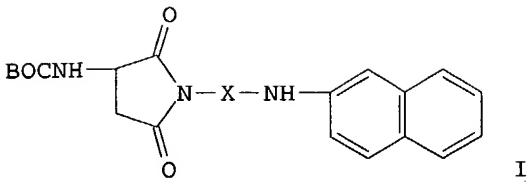

I

AB Peptides containing aspartic acid β-phenacyl ester residues, which do not cyclize under conditions of acidolysis, underwent ring closure to the corresponding succinimido derivs. under basic conditions. When the Cl+ salt of BOC-Asp-Gly-NHNA (BOC = Me3CO2C, NA = β-naphthyl) was esterified with BrCH2COPh, succinimido peptide I (X = Gly) was obtained by cyclization of BOC-Asp(OCH2COPh)-Gly-NHNA. BOC-Asp(OCH2COPh)-Val-NHNA was also prepared and cyclized to I (X = Val) under basic conditions.

AN 89:129915 CA

TI Side reactions in peptide synthesis. 8. On the phenacyl group in the protection of the β-carboxyl function of aspartyl residues

AU Bodanszky, Miklos; Martinez, Jean

CS Dep. Chem., Case Western Reserve Univ., Cleveland, OH, USA

SO Journal of Organic Chemistry (1978), 43(15), 3071-3
CODEN: JOCEAH; ISSN: 0022-3263

DT Journal

LA English

L4 ANSWER 7 OF 9 CA COPYRIGHT 2004 ACS on STN

AB The 1,5-diazabicyclo[4.3.0]non-5-ene and/or 1,8-diazabicyclo[5.4.0]undec-7-ene salts of Me3CO2C-X-OH [X = Gly, Ala, Val, Ile, Tyr(CH2Ph), Arg(SO2C6H4Me-p), Gly-Ile, Trp-Gly], PhCH2O2C-Leu-Ala-OH, PhCH2O2C-Val-Phe-Gly-OH, and p-(O2N)C6H4CH2O2C-Y(OCH2C6H4NO2-p)-OH (Y = Asp, Glu) were esterified to chloromethylated styrene-divinylbenzene polymer in 59-100% yields at 50° for 28 h. The above procedure for the incorporation of N-protected peptides onto the resin did not cause racemization.

AN 87:102642 CA

TI An improved attachment of N-protected amino acid and peptide to chloromethylated polystyrene-divinylbenzene resin

AU Suzuki, Kenji; Endo, Nobuyoshi

CS Tohoku Coll. Pharm., Sendai, Japan

SO Chemical & Pharmaceutical Bulletin (1977), 25(5), 1143-6
CODEN: CPBTAL; ISSN: 0009-2363

DT Journal

LA English

L4 ANSWER 8 OF 9 CA COPYRIGHT 2004 ACS on STN

AB Different published observations of the authors (CA 56, 12153f; 58, 3645e) on the separation of carnitine (I) from possible precursors of I, including 4-aminobutyric acid (II) and some of its hydroxylated and N-methylated derivs., have been reviewed and discussed. In ion-exchange chromatography a satisfactory separation of II from I could not be obtained on a Dowex 50 resin using HCl as eluant because methylation of amino group increases the nonionic adsorption to the resin and, furthermore, the methylated amino group would be expected to be less hydrated than the unsubstituted amino group, as a consequence of which the smaller ions would be held more firmly to the resin by ionic force. Hence an ion-exchange resin with another polarity of the skeleton such as a sulfonated phenolic resin, e.g. Duolite C 3 had been recommended. Thin-layer chromatography has been found to be very convenient to use for a rapid semiquant. determination of the emerging compds. and for their identification.

AN 63:89255 CA

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OREF 63:16454h,16455a-b
TI Separation of carnitine from related compounds by ion-exchange and thin-layer chromatography
AU Lindstedt, Goran; Lindstedt, Sven
CS Karolinska Inst., Stockholm
SO Recent Res. Carnitine, Its Relation Lipid Metab., Papers Symp., Cambridge, Mass. (1965), Volume Date 1964 11-21
DT Journal
LA English

L4 ANSWER 9 OF 9 CA COPYRIGHT 2004 ACS on STN
AB A mixture of 60 g. p-toluene-sulfonic acid monohydrate, 40 g. L-aspartic acid, and 100 mL. benzyl alc. was refluxed with stirring for 18 h. H2O formed was removed through a Dean-Stark separator. Cooling in ice gave 74% dibenzyl L-aspartate p-toluenesulfonate (I), m. 157-8° (aqueous EtOH), [α]25D 1° (EtOH). Similarly prepared were: dibenzyl L-glutamate p-toluenesulfonate (88%), m. 139.5-41.5° (H2O); γ-benzyl L-glutamate p-toluenesulfonate, m. 147-53° (EtOH-Et2O); L-leucine benzyl ester p-toluenesulfonate (62%), m. 211.5-12.5° (H2O). I (100 g.) in 500 mL. Et2O shaken with 45 g. cold Na2CO3 and 100 mL. H2O gave 88% dibenzyl L-aspartate (II), oil; HCl **salt** (60%) m. 129.5-30° (MeOH-Et2O), [α]25D 1° (EtOH). Likewise prepared were: dibenzyl L-glutamate HCl **salt**, m. 99-100°, [α]25D 9° (HCl), and γ-benzyl L-glutamate (43%), m. 162-4°, [α]25D 19° (AcOH). II on long standing deposited 3,6-bis(benzyloxycarbonyl)-2,5-piperazinedione, m. 157-8° (EtOH). L-Aspartic acid (66.5 g.), 500 mL. benzyl alc., and 50 mL. concentrated H2SO4 was kept 20 h. at room temperature and then basified with 200 mL. C5H5N in 1 l. EtOH. The precipitate was filtered off to give 63% β-benzyl L-aspartate, m. 211.5-12.5° (decomposition) (aqueous C5H5N), [α]25D 27° (HCl). Freshly prepared II (9.4 g.), 50 mL. Et2O, 1.9 g. Na2CO3, and 4.5 mL. H2O were stirred with dropwise addition of β-carbomethoxypropionyl chloride in 50 mL. Et2O for 30 min. at 15-17°. After addnl. stirring for 30 min., the Et2O layer was separated, dried (Na2SO4), and concentrated to give 71% N-(β-carbomethoxypropionyl)-L-aspartic acid dibenzyl ester, m. 57-8° (petr. ether). Similarly prepared was 90% N-(β-carbobenzyloxypropionyl)-L-aspartic acid dibenzyl ester (III), m. 70-1.5°. II (28.8 g.), 9 g. succinic anhydride, and 300 mL. CHCl3 heated 30 min. gave 96% N-(β-carboxypropionyl)-L-aspartic acid dibenzyl ester (IV), m. 97-8° (CCl4). III and IV on catalytic hydrogenation sep. gave N-(β-carboxypropionyl)-L-aspartic acid, oil; solid tri-Me ester; tris(p-bromophenacyl) ester m. 138-9° (decomposition) (EtOH); triamide m. 220.5-21° (decomposition) (H2O). II (4.85 g.), 2.3 g. phthalic anhydride, 0.5 mL. Et3N, and 100 mL. PhMe were heated for 3.5 h. to give 6.3 g. dibenzyl N-phthaloyl-L-aspartate, oil, which on catalytic hydrogenation gave 3.7 g. N-phthaloyl-L-aspartic acid, m. 223-6° (H2O), [α]25D -39° (EtOH). Use of HCONMe2 or AcOH gave the DL-ester. Similarly prepared were: 68.5% N-phthaloyl-L-glutamic acid, m. 158-60° (H2O), [α]25D -45° (EtOH); 38% N-phthaloyl-L-leucine, m. 119-21° (aqueous MeOH), [α]25D -24° (EtOH); and 92.5% di-Et N-phthaloyl-L-aspartate, [α]25D -45° (EtOH).
AN 60:9998 CA
OREF 60:1831d-h
TI Some derivatives of aspartic and glutamic acids
AU Bose, Ajay K.; Strube, Richard E.
CS Upjohn Co., Kalamazoo, MI
SO Journal of Pharmaceutical Sciences (1963), 52(9), 847-51
CODEN: JPMSAE; ISSN: 0022-3549
DT Journal

10484927

LA Unavailable
OS CASREACT 60:9998